201-16644B

IUCLID

Data Set

Existing Chemical	:	ID: 298-06-6
CAS No.	:	298-06-6
EINECS Name	:	O,O-diethyl hydrogen phosphorodithioate
EC No.	:	206-055-9
Molecular Formula	:	C4H11O2PS2

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	06.08.2007

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	06.08.2007
Status	:	
Memo	:	Bayer CropScience
Printing date	:	30.08.2007
Revision date	:	
Date of last update	:	30.08.2007
Number of pages	:	39
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	importer of product
Name	:	Bayer Corporation
Contact person	:	
Date	:	
Street	:	100 Bayer Road, Building #5
Town	:	PA 15205-9741 Pittsburgh
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

18.08.2007

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	Phosphorodithioic acid, O,O-diethyl ester
Smiles Code	:	O(P(OCC)(S)=S)CC
Molecular formula	:	C4 H11 O2 P1 S2
Molecular weight	:	186.23
Petrol class	:	

18.08.2007

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for marketed substance
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	colorless to blue-green
Odour	:	

18.08.2007

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Diethyl dithiophosphate

08.08.2007

Diethyl phosphorodithioate

08.08.2007

Diethyl phosphorodithioic acid

08.08.2007

Dithiophosphoric acid O,O-diethyl ester

11.11.2003

Dithiophosphoric acid, O,O-diethyl ester

08.08.2007

Kyselina O,o-diethyldithiofosforecna (Czech)

08.08.2007

Kyselina O,O-diethyldithiofosforecna (Czech)

08.08.2007

O,O'-Diethyl hydrogen dithiophosphate

08.08.2007

O,O-Diethyl dithiophosphate

08.08.2007

O,O-Diethyl dithiophosphoric acid

08.08.2007

O,O-Diethyl hydrogen phosphorodithioate

08.08.2007

O,O-Diethyl phosphorodithioate

08.08.2007

O,O-Diethyl-S-hydrogen phosphorodithioate

08.08.2007

Phosphonodithioic acid, O,O-diethyl ester

08.08.2007

Phosphorodithioate, diethyl-

08.08.2007

Phosphorodithioic acid, O,O-diethyl ester

08.08.2007

Phosphorodithioic acid, O,o-diethyl ester

08.08.2007

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search : Internal and External
Chapters covered : 3, 4, 5
Date of search : 08.08.2007

18.08.2007

1.13 REVIEWS

2.1 MELTING POINT

Value : -10 °C
Sublimation :
Method : other
Year : 2007
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Calculated data is appropriate when the melting point data is under 0 °C.
Result : Experimental Database Structure Match
Reliability : (2) valid with restrictions
Technical discussion
Flag : Critical study for SIDS endpoint
30.08.2007 (4)

2.2 BOILING POINT

Value : 105 - 108 °C at 20 hPa
Decomposition : yes
Method : other: no data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Decomposition at temperatures > 150 degree C
Reliability : (4) not assignable
Internal company data
18.08.2007 (10)

2.3 DENSITY

Type : density
Value : 1.17 g/cm³ at 20 °C
Method : other: no data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (4) not assignable
Internal company data
18.08.2007 (10)

Type : relative density
Value : 1.111 at °C
Method : other: no data
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Reliability : (4) not assignable
No additional details available
18.08.2007

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .077 hPa at 25 °C
Decomposition :
Method : other (calculated): MPBPWIN (v1.41)
Year : 2007
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : MPBPWIN (v1.42) Program
==========
Experimental Database Structure Match:
Name : O,O-Diethyl dithiophosphate
CAS Num : 000298-06-6
Exp MP (deg C): -10
Exp BP (deg C): ---
Exp VP (mm Hg): ---

SMILES : O(P(OCC)(S)=S)CC
CHEM : Phosphorodithioic acid, O,O-diethyl ester
MOL FOR: C4 H11 O2 P1 S2
MOL WT : 186.23

Result : MPBPWIN (v1.42) Program Results:
==========
---- SUMMARY MPBPWIN v1.42 ----------

Boiling Point: 235.63 deg C (Adapted Stein and Brown Method)

Melting Point: -143.77 deg C (Adapted Joback Method)
Melting Point: 23.92 deg C (Gold and Ogle Method)
Mean Melt Pt : -59.92 deg C (Joback; Gold,Ogle Methods)
Selected MP: -59.92 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 235.63 deg C (estimated))
(MP not used for liquids)
VP: 0.0611 mm Hg (Antoine Method)
VP: 0.0554 mm Hg (Modified Grain Method)
VP: 0.0957 mm Hg (Mackay Method)
Selected VP: 0.0583 mm Hg (Mean of Antoine & Grain methods)

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
08.08.2007 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : 1.17 at 25 °C
pH value :
Method : other (calculated)
Year :

GLP : no
Test substance : as prescribed by 1.1 - 1.4

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
08.08.2007 (1)

Partition coefficient : octanol-water
Log pow : 2.24 at 25 °C
pH value :
Method : other (calculated)
Year : 2007
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 2.24

SMILES : O(P(OCC)(S)=S)CC
CHEM : Phosphorodithioic acid, O,O-diethyl ester
MOL FOR: C4 H11 O2 P1 S2
MOL WT : 186.23

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	2	-CH2- [aliphatic carbon]	0.4911	0.9822
Frag	1	S=P [thio=phosphorus]	-0.6587	-0.6587
Frag	2	-O-P [aliphatic attach]	-0.0162	-0.0324
Frag	1	-S-P [sulfur, phosphorus attach]	0.6270	0.6270
Const		Equation Constant		0.2290

Log Kow = 2.2417

Result : KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 2.24

SMILES : O(P(OCC)(S)=S)CC
CHEM : Phosphorodithioic acid, O,O-diethyl ester
MOL FOR: C4 H11 O2 P1 S2
MOL WT : 186.23

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE

Frag | 2 | -CH3 [aliphatic carbon] | 0.5473 | 1.0946
Frag | 2 | -CH2- [aliphatic carbon] | 0.4911 | 0.9822
Frag | 1 | S=P [thio=phosphorus] |-0.6587 | -0.6587
Frag | 2 | -O-P [aliphatic attach] |-0.0162 | -0.0324
Frag | 1 | -S-P [sulfur, phosphorus attach] | 0.6270 | 0.6270
Const | | Equation Constant | | 0.2290

				Log
				Kow = 2.2417

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
08.08.2007 (4)

Partition coefficient :
Log pow : at 23 °C
pH value :
Method : other (measured)
Year : 1976
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : The solvent distribution of diethylphosphorodithioic acid was investigated at room temperature (22-23 degree C) by using 100 ml separation funnels: 10 ml of aqueous solution of 1 M ionic strength were shaken with 10 ml of organic solvent (butanol or benzene) containing known amounts of test substance. After 20 minutes the phases were separated.
The concentration of test substance was determined by iodometric titration or potentiation titration with AgNO3. The volume changes caused by reciprocal solubility in the water-benzene can be neglected. For the water-butanol system, volume corrections were made.
Result : pH50 logP pKa
water/benzene system: 0.30 0.37 -0.07
water/n-butanol s (MISSING DATA HERE)
Test substance : diethylphosphorodithioic acid; purity not noted
Reliability : (2) valid with restrictions
Published data
08.08.2007 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : not soluble
Stable :
Deg. product :
Method : other: no data

Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable Internal company data

22.08.2007 (10)

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	1976
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The solvent distribution of diethylphosphorodithioic acid was investigated at room temperature (22-23 degree C) by using 100 ml separation funnels: 10 ml of aqueous solution of 1 M ionic strength were shaken with 10 ml of organic solvent (butanol or benzene) containing known amounts of test substance. After 20 minutes the phases were separated. The concentration of test substance was determined by iodometric titration or potentiation titration with AgNO3. For the water-butanol system, volume corrections were made.
Result	:	water/n-butanol system: pH50 = 0.70 log P = 0.55 pKa = 0.15
Reliability	:	(3) invalid Does not meet criteria of today's current guidelines

22.08.2007 (2)

Solubility in	:	other: benzene
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	1976
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The solvent distribution of diethylphosphorodithioic acid was investigated at room temperature (22-23 degree C) by using 100 ml separation funnels: 10 ml of aqueous solution of 1 M ionic strength were shaken with 10 ml of organic solvent (butanol or benzene) containing known amounts of test substance. After 20 minutes the phases were separated. The concentration of test substance was determined by iodometric titration or potentiation titration with AgNO3. The volume changes caused by reciprocal solubility in the water-benzene can be neglected.

Result : water/benzene system:
pH50 = 0.30
log P = 0.37
pKa = -0.07
Reliability : (3) invalid
Does not meet criteria of today's current guidelines

22.08.2007 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

Method :
Year : 1960
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : pKa = 1.6
Reliability : (2) valid with restrictions
Published data

30.08.2007 (8)

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.00000000000916 cm³/(molecule*sec)
Degradation	:	50 % after 1.4 hour(s)
Deg. product	:	
Method	:	other (calculated): AOP Program (v1.91
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Method : AOP Program (v1.92)

==========

SMILES : O(P(OCC)(S)=S)CC
CHEM : Phosphorodithioic acid, O,O-diethyl ester
MOL FOR: C4 H11 O2 P1 S2
MOL WT : 186.23

Result : AOP Program (v1.92) Results:

==========

SUMMARY (AOP v1.92): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 38.6286 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 53.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 91.6286 E-12 cm3/molecule-sec
HALF-LIFE = 0.117 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 1.401 Hrs
---------- SUMMARY (AOP v1.91): OZONE REACTION

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi): 2.36E-005
(Junge,Mackay)
Note: the sorbed fraction may be resistant to
atmospheric oxidation

Reliability	:	(2) valid with restrictions Modeled data
Flag	:	Critical study for SIDS endpoint

08.08.2007 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C

t1/2 pH9 : at °C
Deg. product :
Method : other (calculated)
Year : 2007
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : HYDROWIN Program (v1.67):
==========
SMILES : O(P(OCC)(S)=S)CC
CHEM : Phosphorodithioic acid, O,O-diethyl ester
MOL FOR: C4 H11 O2 P1 S2
MOL WT : 186.23
Result : ---------- HYDROWIN v1.67 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant for he type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!!
Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
22.08.2007 (4)

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C

Remark : Hydrolysis is not expected to be a primary route of degradation based on analogy to Disulfoton (CAS 298-04-4). Disulfoton is stable to hydrolysis at 20 oC at pH 5, 7, and 9, but hydrolyzes more rapidly at higher temperatures. Estimated hydrolysis half-lives for Disulfoton were 103 days at 25 ºC and pH 7 (Ellington et al. 1988) and 170 days at 11 ºC and pH 7.9 (Wanner et al. 1989).
Reliability : (2) valid with restrictions
22.08.2007 (3) (14) (16)

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method : other
Year : 1997
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : "Allen's" modified method of colorimetry, in aqueous solutions from 0.1 to 7.0 mol/dm3 HCL at 98 degree C.
Remark : Diethyl dithiophosphate in acid media occurs as both conjugate acid species and neutral species. Comparative data support the bimolecular nature of hydrolysis involving attack of water molecule on phosphorus of the diester involving P-O bond fission.
Result : Experimental and Estimated data for the hydrolysis of diethyl dithiophosphate at 98 degree C

HCL (mol/dm3)	Ke x 10e4 (min-1) (experimental)	Ke x 10e4 (min-1) (estimated)
0.1	11.32	12.68
0.2	12.74	12.87
0.5	13.02	13.45

1.0	13.75	14.44
2.0	16.86	16.58
3.0	18.14	18.91
4.0	22.22	21.45
5.0	16.44	16.51
6.0	15.16	14.60
7.0	13.75	13.22

Test substance : diethyl dithiophosphate; BDH quality
Reliability : (3) invalid
Does not meet criteria of current standard guidelines (conducted at 98 deg C)

22.08.2007 (13)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air, water, soil, sediment
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: EPIWIN modelling program
Year : 2007

Method : Level III Fugacity Model :
==========

Chem Name : Phosphorodithioic acid, O,O-diethyl ester
Molecular Wt: 186.23
Henry's LC : 0.000371 atm-m3/mole (Henrywin program)
Vapor Press : 0.0583 mm Hg (Mpbpwin program)
Log Kow : 2.24 (Kowwin program)
Soil Koc : 71.2 (calc by model)

Result : Level III Fugacity Model (Full-Output):
==========

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.879	2.8	1000
Water	30.7	360	1000
Soil	68.3	720	1000
Sediment	0.145	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	9.06e-012	1.71e+003	69.1	57	2.3

Water 2.4e-009 464 241 15.5
8.03
Soil 2.95e-008 517 0 17.2
0
Sediment 2.1e-009 0.244 0.0228 0.00813
0.00076

Persistence Time: 262 hr
Reaction Time: 292 hr
Advection Time: 2.53e+003 hr
Percent Reacted: 89.7
Percent Advected: 10.3

Half-Lives (hr), (based upon Biowin (Ultimate) and
Aopwin):
Air: 2.801
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 2.788 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
08.08.2007 (4)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge
Concentration : 100 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : 1 (±) % after 28 day(s)
Result : other: not readily biodegradable
Deg. product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year : 2002
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : No further details available
Result : Indirect Analysis: BOD= 1%

Direct Analysis TOC = 0%; GC= 1%
Reliability : (2) valid with restrictions
Guideline study; no data regarding GLP
Flag : Critical study for SIDS endpoint
08.08.2007 (12)

Type : aerobic
Inoculum :
Contact time :
Degradation : (±) % after
Result : inherently biodegradable
Deg. product :
Method : other: BIOWIN (v4.01)
Year : 2007
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : BIOWIN (v4.10) Program
==========
SMILES : O(P(OCC)(S)=S)CC
CHEM : Phosphorodithioic acid, O,O-diethyl ester
MOL FOR: C4 H11 O2 P1 S2
MOL WT : 186.23

Result : BIOWIN (v4.10) Program Results:
==========
BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction) : Does Not Biodegrade Fast
Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt	*	Molecular Weight Parameter		-0.0887
Const	*	Equation Constant		0.7475

RESULT	Biowin1 (Linear Biodeg Probability)	0.6589

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
MolWt	*	Molecular Weight Parameter		-2.6444

```
======+=========
  RESULT   |  Biowin2 (Non-Linear Biodeg Probability)   |
     |  0.5901
============+=============================================
+==
======+=========

 A Probability Greater Than or Equal to 0.5 indicates -->
Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT
Biodegrade Fast

------+-----+-------------------------------------------+--
------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION        |
COEFF  |  VALUE
------+-----+-------------------------------------------+--
------+---------
 MolWt|  *  |  Molecular Weight Parameter               |
     | -0.4115
 Const|  *  |  Equation Constant                        |
     |  3.1992
============+=============================================
+==
======+=========
  RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)  |
     |  2.7876
============+=============================================
+==
======+=========

------+-----+-------------------------------------------+--
------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION        |
COEFF  |  VALUE
------+-----+-------------------------------------------+--
------+---------
 MolWt|  *  |  Molecular Weight Parameter               |
     | -0.2687
 Const|  *  |  Equation Constant                        |
     |  3.8477
============+=============================================
+==
======+=========
  RESULT   |   Biowin4 (Survey Model - Primary Biodeg)  |
     |  3.5791
============+=============================================
+==
======+=========

 Result Classification:   5.00 -> hours     4.00 -> days
3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-------------------------------------------+--
------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION        |
COEFF  |  VALUE
------+-----+-------------------------------------------+--
------+---------
 Frag |  2  |  Methyl  [-CH3]                           |
0.0004 |  0.0008
```

```
 Frag |  2  | -CH2-  [linear]                      |
0.0494 |  0.0988
 MolWt|  *  |  Molecular Weight Parameter          |
     | -0.5540
 Const|  *  |  Equation Constant                   |
     |  0.7121
============+=========================================
+==
======+=========
  RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |
     |  0.2578
============+=========================================
+==
======+=========

------+-----+-----------------------------------------+--
------+---------
 TYPE | NUM |      Biowin6 FRAGMENT DESCRIPTION       |
COEFF  |  VALUE
------+-----+-----------------------------------------+--
------+---------
 Frag |  2  |  Methyl  [-CH3]                      |
0.0194 |  0.0389
 Frag |  2  |  -CH2-  [linear]                     |
0.4295 |  0.8590
 MolWt|  *  |  Molecular Weight Parameter          |
     | -5.3761
============+=========================================
+==
======+=========
  RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|
     |  0.1243
============+=========================================
+==
======+=========

 A Probability Greater Than or Equal to 0.5 indicates -->
Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily
Degradable


------+-----+-----------------------------------------+--
------+---------
 TYPE | NUM |      Biowin7 FRAGMENT DESCRIPTION       |
COEFF  |  VALUE
------+-----+-----------------------------------------+--
------+---------
 Frag |  2  |  Methyl  [-CH3]                      |
-0.0796 | -0.1591
 Frag |  2  |  -CH2-  [linear]                     |
0.0260 |  0.0520
 Const|  *  |  Equation Constant                   |
     |  0.8361
============+=========================================
+==
======+=========
  RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)   |
     |  0.7289
============+=========================================
+==
======+=========
```

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Reliability : (2) valid with restrictions
Modeled data

08.08.2007 (4)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	42 day(s) at °C
Concentration	:	
BCF	:	< .5 - 5
Elimination	:	
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	At an exposure concentration of 1 mg/L the BCF < 0.5; at 0.1 mg/L the BCF < 5
Conclusion	:	Low bioaccumulation potential
Reliability	:	(2) valid with restrictions National on-line data base

18.08.2007 (12)

Species	:	other
Exposure period	:	at 25 °C
Concentration	:	
BCF	:	10.62
Elimination	:	
Method	:	other: (calculated) BCF Program (v2.15)
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Modeled data

18.08.2007 (4)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	Oryzias latipes (Fish, fresh water)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LC50	:	440
Limit test	:	no
Analytical monitoring	:	no data
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Although additional details are not available, this study is considered valid as it was conducted as part of a national testing program. Reported as part of a bioaccumulation study
Reliability	:	(2) valid with restrictions National on-line data base
Flag	:	Critical study for SIDS endpoint

22.08.2007 (12)

Type	:	
Species	:	Poecilia reticulata (Fish, fresh water)
Exposure period	:	24 hour(s)
Unit	:	mg/l
LC50	:	79
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable No additional details available

22.08.2007 (10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	24 hour(s)
Unit	:	mg/l
EC50	:	.54
Limit Test	:	no
Analytical monitoring	:	no
Method	:	OECD Guide-line 202
Year	:	1994
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Additional details not available.
Test substance	:	diethyldithiophosphate; purity = 90%; obtained from Aldrich, Germany
Reliability	:	(2) valid with restrictions Guideline study; no data regarding GLP
Flag	:	Critical study for SIDS endpoint

22.08.2007 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	aquatic
Species	:	Photobacterium phosphoreum (Bacteria)
Exposure period	:	30 minute(s)
Unit	:	mg/l
EC10	:	3.13
Analytical monitoring	:	no data
Method	:	other: Microtox assay
Year	:	1994
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The inhibition of bioluminescence was measured according to Beckman Microtox system operating manual (1982) in a saline solution (2% NaCl in water) at a temperature of 15 degrees C, after a 30 minute incubation.
Test substance	:	diethyldithiophosphate; purity = 90%; obtained from Aldrich, Germany
Reliability	:	(3) invalid Does not meet criteria of today's current guidelines

22.08.2007 (7)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1400 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	20
Vehicle	:	
Doses	:	1260, 1580, 2000, and 2510 mg/kg
Method	:	other
Year	:	1979
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Animals were dosed by gavage and observed for mortality and signs of toxicity over a 14-day post-exposure period. Initial and final body weights were recorded. Gross necropsy was performed on all animals.
Result	:	Dose Mortalities/Dosed (mg/kg) Male Females Combined 1,260 0/2 1/3 1/5 1,580 3/3 1/2 4/5 2,000 2/2 3/3 5/5 2,510 3/3 2/2 5/5 Time to Death: one to four days Signs of toxicity: Weight loss (one to four days in survivors); increasing weakness, collapse, and death. Gross necropsy of decedents: Hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation. Gross necropsy of survivors: Viscera appeared normal.
Test substance	:	Diethyl Phosphorodithioic acid (CAS No. 298-06-6); purity not reported
Reliability	:	(2) valid with restrictions Provides basic data
Flag	:	Critical study for SIDS endpoint

22.08.2007 (18)

Type	:	LD50
Value	:	= 398 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	20
Vehicle	:	other: corn oil
Doses	:	316, 398, 501, and 631 mg/kg
Method	:	other
Year	:	1962
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The diluted compound (25% solution in corn oil) was dosed by gavage in Sprague-Dawley strain albino rats. After the approximate Minimum Lethal Dose was determined, groups of male and female rats (total of five rats/dose group) were gavaged in increasing doses at increments of 0.1 fractional log intervals at four levels (316, 398, 501, and 631 mg/kg)

designed to blanket the toxicity range thereby supplying data for the calculation of the LD50 which was done according to a modification of the method of E.J.de Beer.

Observations were made for toxic symptoms and the viscera of the animals that succumbed were examined macroscopically.

Result : Dose Mortality Data (dead/dosed)

(mg/kg)	Male	Female
316	0/2	1/3
398	1/2	1/3
501	1/2	3/3
631	3/3	2/2

Survival time was several hours to three days with most deaths occurring overnight. Toxic symptoms included tremors after several hours, salivation, dyspnea and increasing weakness. At necropsy there was inflammation of the gastric mucosa with renal and liver hyperemia.

LD50 (combined) = 398 mg/kg (CL 330 - 477 mg/kg)

Test substance : purity not reported
Reliability : (4) not assignable
Insufficient data to determine reliability (not sure how long the animals were observed)

22.08.2007 (17)

Type : LD50
Value : = 4510 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: no data
Year : 1986
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Test substance : Phosphorodithioic acid, O,O-diethyl ester; purity not noted
Reliability : (4) not assignable
Insufficient data to determine reliability

22.08.2007 (9)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Value : = 1.64 - 2.48 mg/l
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 60
Vehicle :
Doses : 0.98, 1.02, 10.4, 1.35, 1.60, and 2.10 mg/L
Exposure time : 4 hour(s)
Method : other
Year : 1981
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : Six groups of rats (5/sex/dose) of Sprague-Dawley rats were exposed for 4

hours to an atmosphere of O,O'-Diethyl Phosphorodithioate (ethyl thioacid). The aerosol-vapor atmosphere of ethyl thioacid was produced by metering the liquid from a pressurized tank through a capillary restrictor to a Laskin-style nebulizer located in the top inlet of t glass/stainless steel exposure changes. The concentration of the test material in the chamber was varied by changing the head pressure in the tank and subsequently, the flow rate of the test material to the nebulizer. Four analytical samples and four nominal atmospheric concentration measurements were obtained at approximately one-hour intervals during the exposure. Signs of toxicity were recorded during the exposure, on each hour for three hours following the exposure, and twice daily during a 14-day post-exposure period. Body weights were recorded on Days 1, 7, and 14. All survivors were terminated at the end of the post-exposure period and subjected to a standard macroscopic examination of the tissues from the thoracic, abdominal and cranial cavities.

Cholinesterase inhibition in the red blood cells and plasma was determined in six additional male rats which were exposed with the group of rats at the 0.98 mg/l etyhl thioacid level. These animals were not included in the mortality data used in the probit analysis.

Result **:** Analytical results for the six exposures resulted in a narrow range of concentrations of 0.98 to 2.10 mg/l of vapor/aerosol in air. Nominal concentrations ranged from 2.49 to 8.01 mg/L.

The combined mortality for the six exposure groups was 18 out of 60 (8 males and 10 females), as follows:

Nominal (mg/L)	Analytical (mg/L)	N/A ratio Males	Mortaltiy Females
3.32	0.98	3.39	0/5 1/5
2.49	1.02	2.44	1/5 1/5
5.96	1.04	5.73	1/5 1/5
4.86	1.35	3.60	2/5 1/5
4.95	1.60	3.09	3/5 2/5
8.01	2.10	3.81	1/5 4/5

The gross signs of toxicity observed during the exposures were clear nasal discharge, lacrimation, breathing difficulties, hypoactivity and fur discoloration (fur covered with test material). During the 14-day post-exposure period, hypoactivity, breathing difficulties, chromodacryorrhea around the mouth, nose and eyes, initial loss in body weight, and death were observed. Infrequently during these two weeks, abrasions, edema and swelling about the nose and mouth, wheezing, dehydration, emaciation, clear nasal discharge, lacrimation, piloerection, and tremors were observed. Red blood cell and plasma cholinesterase levels were increased 115% and decreased 30%, respectively, in six male rats exposed to 0.98 mg ethyl thioacid per liter of air.

The most frequent necropsy findings observed in rats, sacrificed either in extremis or sacrificed per design at the end of the post-exposure period, were petechial hemorrhage of the thymus and lungs, alopecia, chromodacryorrhea and abrasions about the mouth and nose.

The mean lethal concentration (LC50) was calculated by Finney's Probit procedure using the total number of exposure groups (6):

Combined sexes:
LC50 = 1.89
95% limits = (1.48-9.41)
LC10 = 0.80

Males:

LC50 = 2.48
95% limits = (1.48 - infinity)
LC10 = 0.69

Females:
LC50 = 1.64
95% limits = (1.28-8.07)
LC10 = 0.87
The LC50 for the males is an extrapolated value, since it exceeded the concentration of the highest exposure level (2.10 mg/L). Under these experimental conditions, higher analytical concentrations could not be obtained.

Test substance : Purity: 85% ethyl thioacid
Conclusion : The body weight data, gross signs of toxicity, cholinesterase and mortality data and necropsy findings suggest that ethyl thioacid when administered by inhalation exposure is of moderate acute toxicity to rats.
Reliability : (2) valid with restrictions
Comparable to guideline; no data on GLP
Flag : Critical study for SIDS endpoint
23.08.2007 (11)

Type : LC50
Value : > .7 mg/l
Species : rat
Strain : Sprague-Dawley
Sex : male
Number of animals : 6
Vehicle :
Doses : 0.7 mg/l
Exposure time : 6 hour(s)
Method : other
Year : 1979
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : Concentration: 0.7 mg/L
Exposure: 6 hrs
Chamber temp: 25 deg C
Chamber humidity: 65%
Post-exposure observation period: 14 day
Result : Mortality: 1/6
1-15 min: Labored breathing, ocular erythema, increasing weakness
15-30 min: tremors, nasal bleeding, one appeared dead in thirty minutes;
After 30 minutes: five appeared normal during the remainder of exposure period
Necropsy of decedent: Hemorrhagic lungs
Necropsy of survivors: Viscera appeared normal
Test substance : Diethyl Phosphorodithioic acid (CAS No. 298-06-6); purity not reported
Reliability : (2) valid with restrictions
Provides basic data
17.08.2007 (18)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 2000 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 4

Vehicle	:	
Doses	:	1000, 2000, 3160, and 5010 mg/kg
Method	:	other
Year	:	1979
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : The test article was applied undiluted. Exposure was for 24 hours. Mortality and signs of toxicity were recorded over a 14-day post-exposure period. Initial and final body weights recorded. Gross necropsy was performed on all animals.

Result :
Dose Mortalities/Dosed
(mg/kg)
1,000: one male dosed-survived; no females dosed
2,000: no males dosed; one female dosed-survived
3,160: one male dosed-died within two days; no females dosed
5,010; no males dosed; one female dosed-dead within one day

Signs of toxicity: Weight loss (two to four days in survivors); increasing weakness, ocular discharge; collapse, and death.
Gross necropsy of decedents: Lung hyperemia, enlarged gall bladder, and darkened spleen.
Gross necropsy of survivors: Viscera appeared normal.

Test substance	:	Diethyl Phosphorodithioic acid (CAS No. 298-06-6); purity not reported
Reliability	:	(2) valid with restrictions Provides basic data
Flag	:	Critical study for SIDS endpoint

22.08.2007 (18)

Type	:	LD50
Value	:	= 415 - mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	female
Number of animals	:	9
Vehicle	:	
Doses	:	251, 398, and 631 mg/kg
Method	:	
Year	:	1962
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Method : After the approximate Minimum Lethal Dose was determined, the undiluted compound was applied in increasing doses at increments of 0.2 fractional log intervals to the closely clipped, intact skin of New Zealand white female rabbits (3 animals/dose group) at three levels (251, 398, and 631 mg/kg) designed to blanket the toxicity range thereby supplying data for calculation of the LD50 which was done according to a modification of the method of E.J. de Beer. The treated areas were covered with plastic strips and the animals placed in wooden stocks for periods up to 24 hours, after which they were placed in individual cages. Observations were made for toxic symptoms and the viscera of the animals that succumbed were examined macroscopically.

Result :
Dose Mortality Data (dead/dosed)
(mg/kg) Female
251 0/3
398 2/3
631 3/3

Survival time was twelve hours to three days. Toxic symptoms included weakness after several hours, lethargy, tremors, and collapse. At necropsy there was pulmonary hyperemia, otherwise there were no visceral changes

of consequence noted.

Approximate LD50 (female) = 415 mg/kg (CL 320-530 mg/kg)

Test substance : purity not reported
Reliability : (4) not assignable
Insufficient data to determine reliability (not sure how long animals were observed)

22.08.2007 (17)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Open
Exposure time : 24 hour(s)
Number of animals : 3
Vehicle :
PDII : 8
Result : highly corrosive
Classification : highly corrosive (causes severe burns)
Method : other
Year : 1962
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : 0.5 ml of undiluted compound was applied to the clipped, intact skin of albino rabbits and removed after 24 hours with soap and warm water. The applied area was covered with plastic strips to retard evaporation. Observations were made over a period of several days for irritation. The data was scored according to the method of Draize.

Result : Animal Numerical Evaluation at the End of (hr)

Number		1	4	24	48	72	120	168
1	2	4	8	8	8	8	8	
2	3	6	8	8	8	8	8	
3	2	5	8	8	8	8	8	
Avg.	2.3	5	8	8	8	8	8	

Slight edema and a whitish appearance developed on the skin within one hour for an average score of 2.3 out of a possible 8. Edema sufficient to outline the treated areas was noted in 4 hours increasing the average score to 5.0. The skin remained whitish, a condition often observed in the first few hours of severe tissue injury. Overnight there was severe swelling and obvious evidence of tissue necrosis resulting in the average maximum score of 8. The destroyed tissue turned red and gradually dried after several days.

The compound was classified as a corrosive skin irritant. The average maximum score was 8.0 out of a possible 8 in 24 hours.

Test substance : purity not reported
Reliability : (2) valid with restrictions
Provides basic data

18.08.2007 (17)

Species : rabbit
Concentration : undiluted
Exposure : no data

Exposure time	:	24 hour(s)
Number of animals	:	6
Vehicle	:	
PDII	:	
Result	:	highly corrosive
Classification	:	highly corrosive (causes severe burns)
Method	:	other: F.H.S.A.
Year	:	1979
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	0.5 ml of undiluted compound was applied. 24-hr exposure Scored for erythema and edema (maximum score of 8) Observed for at least 10 days.
Result	:	Maximum score of 8.0 recorded in all animals within 24 hours. Loosening about edges of scab in 7 to 10 days showed the depth of the injury.
Test substance	:	Diethyl Phosphorodithioic acid (CAS No. 298-06-6); purity not reported
Reliability	:	(2) valid with restrictions Provides basic data

18.08.2007 (18)

Species	:	rabbit
Concentration	:	500 mg
Exposure	:	Occlusive
Exposure time	:	24 hour(s)
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	slightly irritating
Classification	:	
Method	:	Draize Test
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	Phosphorodithioic acid, O,O-diethyl ester; purity not noted
Reliability	:	(4) not assignable Insufficient data to determine reliability

22.08.2007 (9)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure time	:	
Comment	:	other: rinsed after 4 seconds, 10 seconds, or 24 hours
Number of animals	:	3
Vehicle	:	
Result	:	highly corrosive
Classification	:	risk of serious damage to eyes
Method	:	other
Year	:	1962
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	0.1 ml of undiluted sample was placed in the conjunctival sac of the right eye of each of three albino rabbits and observations made over a period of several days of inflammation. The eyes were rinsed with warm isotonic

saline solution in animal #1 after 24 hours, in animal #2 after ten seconds, and in animal #3 after 4 seconds.

Result : Animal Numerical Evaluation at the End of (hr)

Number	1	4	24	48	72	120	168
1	110	110	110	110	110	110	
2	110	110	110	110	110	110	
3	110	110	110	110	110	110	
Avg.	110	110	110	110	110	110	

Where:
Animal #1: 24 hour rinse
Animal #2: 10-second rinse
Animal #3: 4-second rinse

The animals jumped immediately upon application and the cornea became opaque even in the eye of the animal with the 4 second exposure. There was rapid edema extending for a considerable area around the eye resulting in the lids being closed in all instances in less than one hour. Copious lacrimation, beefy red conjunctivae and invisible iris indicating loss of vision produced the maximum score of 110 for all three exposures.

Test substance : purity not reported
Conclusion : This compound was determined to be a corrosive eye irritant. The maximum score was 110 out of a possible 110 in one hour. A four second exposure produced loss of sight.
Reliability : (2) valid with restrictions
Provides basic data

18.08.2007 (17)

Species :
Concentration : .1 mg
Dose :
Exposure time : 24 hour(s)
Comment :
Number of animals :
Vehicle :
Result : highly irritating
Classification :
Method :
Year :
GLP : no data
Test substance : other TS: Phosphorodithioic acid, O,O-diethyl ester; purity not noted

Test substance : Phosphorodithioic acid, O,O-diethyl ester; purity not noted
Reliability : (4) not assignable
Insufficient data to determine reliability

22.08.2007 (9)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA1535, TA1537, TA1538, TA98 and TA100
Test concentration : 50, 100, 250, 500, and 1000 ug/plate
Cycotoxic concentr. : >=3333.3 ug/plate
Metabolic activation : with and without

Result : positive
Method : other: Ames test
Year : 1986
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The mutagenicity of O,O-diethyl phosphorodithioate was evaluated in Salmonella tester strains TA98, TA100, TA1535, TA1537 and TA1538 (Ames test), both in the presence and absence of Aroclor-induced rat liver S9 metabolic activation.

Preliminary toxicity determination: The Salmonella/mammalian microsome mutagenicity assay is divided into two phases. The first phase, the preliminary toxicity determination, is used to establish the dose range over which the test article will be assayed. The second phase is the mutagenicity assay of the test article. In the preliminary assay, strain TA 100 was used and the test article was diluted in DMSO and dosed at 10, 33.3, 66.7, 100, 333.3, 666.7, 1,000, 3333.3, 6666.7, and 10,000 ug/plate with and without metabolic activation.

Definitive assay:
Five doses of the test article in DMSO (50, 100, 250, 500, and 1000 ug/plate) were plated with all five tester strains with and without metabolic activation. All solvent controls and test article doses were plated in triplicate. The plates were incubated for 48-72 hours at 37 +/- 3 deg C.

Positive controls were included:
Without S9 activation: Sodium azide (5 ug/plate); 9-Aminoacridine (75 ug/plate); 2-Nitrofluorene (5 ug/plate)
With S9 activation: 2-Anthramine (4 ug/plate)

Result : Preliminary assay: The results of the preliminary toxicity determination indicated that the appropriate maximum dose level to be tested in the mutagenicity assay would be 1000 ug/plate with and without metabolic activation.

Definitive assay: Positive control plates, TA 1537, and plates with greater than 500 colonies per plate were hand counted and manually entered into the computer. The other experimental plates were machine counted and automatically entered into the computer. Mean summary data are presented below:

Dose	S9	Salmonella strains (revertants/plate)				
		TA1535	TA1537	TA1538	TA98	TA100
50	(-)	184*	5	--	18	373
100	(-)	304*	7	--	20	417
250	(-)	644*	7	--	17	654*
500	(-)	902*	7	--	17	986*
1000	(-)	1189*	5	--	16	1378*
50	(+)	15	9	--	31	274
100	(+)	17	8	--	35	272
250	(+)	18	9	--	33	274
500	(+)	74*	10	--	23	246
1000	(+)	335*	9	--	28	366

where * = significant increase over solvent control

A dose response increase or 5.8 fold over the appropriate solvent control was observed in TA 100 without metabolic activation. Exposure of TA1535 also resulted in a dose response increase of 41 fold over the appropriate solvent control without metabolic activation, and a 23.9 fold increase with metabolic. TA1538 was contaminated, so a repeat mutagenicity was performed with this strain. Tester strain TA1535 was also repeated.

Repeat assay: For the repeat mutagenicity assay all plates were hand counted and manually entered into the computer. Mean summary data for the repeated study are provided below:

Dose (ug/plate)	S9	Salmonella strains (revertants/plate) TA1535	TA1538
50	(-)	226*	13
100	(-)	428*	16
250	(-)	664*	14
500	(-)	852*	17
1000	(-)	986*	15
50	(+)	16	28
100	(+)	14	22
250	(+)	17	23
500	(+)	80*	22
1000	(+)	320*	22

No increase was observed in tester strain TA1538 either with or without metabolic activation. A positive dose response was again observed in TA1535 resulting in a 32.9 fold increase without metabolic activation, and a 21.3 fold increase with metabolic activation over the appropriate solvent.

Test substance : O,O-diethyl phosphorodithioate; Lot number KHB-3;39; purity > 90%
Conclusion : Under the conditions of the study, the test material did cause a positive response in TA1535 both with and without metabolic activation, and in TA100 without metabolic activation by Aroclor-induced rat liver microsomes.
Reliability : (1) valid without restriction
Guideline study
Flag : Critical study for SIDS endpoint
18.08.2007 (5)

Type : Ames test
System of testing : Salmonella typhimurium TA1535, TA1537, TA1538, TA98 and TA100
Test concentration : 250, 500, 1000, 2500, and 5000 ug/plate
Cycotoxic concentr. : > 5000 ug/plate
Metabolic activation : with and without
Result : positive
Method : other
Year : 1986
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : The mutagenicity of O,O-diethyl phosphorodithioate was evaluated in Salmonella tester strains TA98, TA100, TA1535, TA1537 and TA1538 (Ames test), both in the presence and absence of Aroclor-induced rat liver S9 metabolic activation. O,O-diethyl phosphorodithioate, diluted in DMSO, was tested at concentrations of 250, 500, 1000, 2500, and 5000 ug/plate using the plate incorporation technique.

Positive controls were included:

Without S9 activation: Sodium azide (5 ug/plate); 9-Aminoacridine (75 ug/plate); 2-Nitrofluorene (5 ug/plate)
With S9 activation: 2-Anthramine (4 ug/plate)

Result : The following table identifies the positive responses noted in the study. The number of total revertant colonies/plate could not be read accurately from the available microfiche of the study.

Dose	S9	Salmonella strains (total revertant colonies/plate) TA1535	TA1537	TA1538	TA98	TA100

250	(-)	*	*
500	(-)	*	*
1000	(-)	*	*
2500	(-)	*	*
5000	(-)	*	*
250	(+)	*	
500	(+)	*	
1000	(+)	*	
2500	(+)	*	
5000	(+)	*	

* = positive response
DTA induced a positive mutagenic response in strain TA100 without activation and in strain TA1535, both with and without activation. All other assays were negative.

Reliability : (2) valid with restrictions
Standard method; no data regarding GLP

17.08.2007 (6)

Type : Ames test
System of testing : Salmonella typhimurium TA1538, TA98, TA1535, TA100, TA1537
Test concentration : 10, 20 and 50 ug/plate without activation
Cycotoxic concentr. : no data
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1982
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Bacterial strains were received from Professor B.N. Ames, University of California, US.
Concentration/plate not available for system in the presence of metabolic activation. Cytotoxic concentration not reported.
Test substance : O,O-diethyldithiophosphate; purity not noted
Reliability : (4) not assignable
Insufficient data to determine reliability

22.08.2007 (15)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

Endpoint : Heptotoxicity

Study descr. in chapter	:	
Reference	:	
Type	:	other: in vitro
Species	:	other: horse
Sex	:	
Strain	:	
Route of admin.	:	
No. of animals	:	
Method	:	
Year	:	1994
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : To 1.0 ml of enzyme solution (containing 15 ug horse blood serum in 70 mM phosphate buffer pH 6.5) 1.0 ml of varying aqueous dilutions of insecticide solution was added, mixed, and incubated for 5 minutes at 20 degree C. After addition of 0.5 ml substrate solution (containing 4.0 mg butyrylthiocholin iodide in 70 mM phosphate buffer pH 6.5) the mixture was incubated for 5 minutes at 37 degree C in a water bath. Then 1.0 ml staining solution (containing 0.1 mg dichlorophenolindophenol in 70 mM phosphate buffer pH 6.5) was added and incubated at 37 degree C. After 5 minutes, the color was assessed visually - a dark blue color indicates total inhibition of AChE.

Result : > 1000 mg/l of dithiophosphate was needed for complete inhibition of AChE

Test substance : diethyldithiophosphate; purity = 90%; obtained from Aldrich, Germany

18.08.2007 (7)

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Advanced Chemistry Development (ACD) (no date) Software Solaris v.4.67 (copyright 1994-2002 ACD)

(2) Curtui M, Marcu G, and Haiduc I. (1976). Solvent Extraction of Uranium (VI) with dialkylphosphorodithioic acids (III). Studia Univ. Babes-Bolyai Chemia. 21:74-79

(3) Ellington JJ, Stancil FE, Payne WD, et al. 1988. Measurement of hydrolysis rate constants for evaluation of hazardous waste land disposal: Vol. 3. Data on 70 chemicals. Engineering Research Laboratory, U.S. Environmental Protection Agency, Athens, GA. EPA/600/S3-88-028. NTIS PB38-234842/AS. Cited in ATSDR Toxicological Profile for Disulfoton (1995) http://www.atsdr.cdc.gov/toxprofiles/tp65.html#bookmark12

(4) EpiWin v. 3.11 (2007)

(5) FMC Corporation (1986) O,O-DIETHYL PHOSPHORODITHIOATE: Salmonella/Mammalian-Microsome Plate Incorporation Mutagenicity Assay (Ames Test). Study Number A85-1676. Fiche Number: 0000465-2 Cited in NISC BiblioLine

(6) FMC Genetic Toxicology Laboratory (1986) O,O-Diethyl Phosphorodithioate: Preliminary results for a second Ames Salmonella/microsome Mutagenicity Test with A New Sample of O,O-Diethyl Phosphorodithioate w/Letter and EPA Acknowledgement Letter. EPA Document No. FYI-OTS-0386-0465, Fiche No. OTS0000465-0. Cited in NISC BiblioLine

(7) Galli R, Rich H W, Scoltz R. (1994). Toxicity of organophosphate insecticides and their metabolites to the water flea, Daphnia magna, the Microtox test and an acetylcholinesterase inhibition test. Aquatic Tox. 30:259-269.

(8) KABACHNIK M.I., T. A. MASTRUKOVA, A. E. SHIPOV and T. A. MELENTYEVA (1960) THE APPLICATION OF THE HAMMETT EQUATION TO THE THEORY OF TAUTOMERIC EQUILIBRIUM THIONE-THIOL EQUILIBRIUM, ACIDITY, AND STRUCTURE OF PHOSPHORUS THIO-ACIDS. Tetrahedron. 1960. Vol. 9. pp. 10 to 28.

(9) Marhold, J. 1986. "Prehled Prumyslove Toxicologie; Organicke Latky." Prague, Czechoslovakia, Avicemun. as reported in "Registry of Toxic Effects of Chemical Substances" compiled by the National Institute for Occupational Safety and Health of the U.S. Department of Health and Human Services. 1993-2003.

(10) Merck KGaA (no date) Frankfurter Str. 250, D-64293 Darmstadt, Germany. www.chemdata.de/

(11) MONSANTO AGRIC CO (1981) O,O-DIETHYL PHOSPHORODITHIOATE INITIAL SUBMISSION: ACUTE INHALATION LC50 OF O,O'-DIETHYL PHOSPHORODITHIOATE (ETHYL THIOACID) IN SPRAGUE-DAWLEY RATS (FINAL REPORT) WITH ATTACHMENTS AND COVER LETTER DATED 040692. Cited in NISC BiblioLine.

(12) National Institute of Technology and Evaluation (NITE) (2002) Biodegradation and Bioconcentration of Existing Chemical Substances under the Chemical Substances Control Law http://www.safe.nite.go.jp/data/sougou/pk_e_search_frm.html? cs_no=298-06-6

(13) Patil R, Shinde CP, Samadhia A. (1997). Kinetics and mechanism of hydrolysis of diethyl dithiophosphate in Acid Media. Asian J. Chemistry. 9(3):407-410.

(14) Patterson, M (2003) Disulfoton Analysis of Risks to Endangered and Threatened Salmon and Steelhead. USEPA, Environmental Field Branch Office of Pesticide Programs. http://www.epa.gov/oppfead1/endanger/effects/disulfoton-analysis.pdf

(15) Szarapinska-Kwaszewska, J. and Rozalska, M. (1982). Study of environmental carcinogens. I. Mutagenic activity of organophosphate pesticides. Inst. Patol., Akad. Med., Lodz, Poland. Bromatol. Chem. Toksykol. 15(1-2):89-93

(16) Wanner U, Egli, T., Fleischmann T, et al. 1989. Behavior of the insecticides disulfoton and thiometon in the Rhine River.A chemodynamic study. Environmental Science and Technology 23:1232-1242. Cited in ATSDR Toxicological Profile for Disulfoton (1995) http://www.atsdr.cdc.gov/toxprofiles/tp65.html#bookmark12

(17) Younger Laboratories (1962) O,O-DIETHYL PHOSPHORODITHIOATE INITIAL SUBMISSION: TOXICOLOGICAL INVESTIGATION OF O,O-DIETHYLPHOSPHORODITHIOIC ACID ETHYL THIOACID WITH COVER LETTER DATED 061092. Fiche No. 0536767 and No. 0543125 Cited in NISC BiblioLine

(18) Younger Laboratories (1979) O,O-DIETHYL PHOSPHORODITHIOATE INITIAL SUBMISSION: LETTER FROM MONSANTO CO TO US EPA SUBMITTING ENCLOSED SUMMARY CONCERNING DIETHYL PHOSPHORODITHIOC ACID ACUTE EYE AND SKIN IRRITATION STUDIES WITH ATTACHMENT. Fiche No. 0543123 Document Number: 88-920004808 Cited in NISC BiblioLine

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-16644C

IUCLID

Data Set

Existing Chemical	:	ID: 3338-24-7
EINECS Name	:	sodium O,O-diethyl dithiophosphate
EC No.	:	222-079-2
Molecular Formula	:	C4H11O2PS2.Na

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	06.08.2007

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	06.08.2007
Status	:	
Memo	:	Bayer CropScience
Printing date	:	10.10.2007
Revision date	:	
Date of last update	:	10.10.2007
Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	importer of product
Name	:	Bayer Corporation
Contact person	:	
Date	:	
Street	:	100 Bayer Road, Building #5
Town	:	PA 15205-9741 Pittsburg
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

09.08.2007

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	Phosphorodithioic acid, O,O-diethyl ester, sodium salt
Smiles Code	:	CCOP(S[Na])(=S)OCC
Molecular formula	:	C4 H10 O2 P1 S2 Na1
Molecular weight	:	209
Petrol class	:	

09.08.2007

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for marketed substance
Substance type	:	other: organic salt
Physical status	:	liquid
Purity	:	
Colour	:	colorless-yellow
Odour	:	

09.08.2007 (1)

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

O,O-Diethyl sodium phosphorodithioate

09.08.2007

O,o-Diethyldithiofosforecnan sodny (Czech)

09.08.2007

O,O-Diethyldithiofosforecnan sodny (Czech)

09.08.2007

Phosphorodithioic acid, O,o-diethyl ester, sodium salt

09.08.2007

Sodium diethyl phosphorodithioate

09.08.2007

Sodium O,O-diethyl dithiophosphate

09.08.2007

Sodium O,O-diethyl phosphorodithioate

09.08.2007

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search : External
Chapters covered : 3, 4, 5
Date of search : 08.08.2007

09.08.2007 (9)

1.13 REVIEWS

2.1 MELTING POINT

Value	:	182 - 183 °C
Sublimation	:	
Method	:	
Year	:	1982
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Melting point not applicable; substance is a liquid at ambient temperature
Result	:	Freezing point
Reliability	:	(2) valid with restrictions Published data
Flag	:	Critical study for SIDS endpoint

10.10.2007 (7)

2.2 BOILING POINT

Decomposition	:	yes
Method	:	
Year	:	1991
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable Internal company data

09.08.2007 (1)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .0000000395 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	MPBPWIN (v1.42) Program: ========== Experimental Database Structure Match: no data SMILES : CCOP(S[Na])(=S)OCC CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt MOL FOR: C4 H10 O2 P1 S2 Na1 MOL WT : 208.21
Remark	:	=VP = 2.06E-008 mm Hg = 3.946342E-06 Pa = 3.95E-08 hPa
Result	:	---------- SUMMARY MPBPWIN v1.42 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 480.00 deg C (estimated))
(Using MP: 90.27 deg C (estimated))
VP: 5.99E-010 mm Hg (Antoine Method)
VP: 2.06E-008 mm Hg (Modified Grain Method)
VP: 4.2E-008 mm Hg (Mackay Method)
Selected VP: 2.06E-008 mm Hg (Modified Grain Method)
Subcooled liquid VP: 8.76E-008 mm Hg (25 deg C, Mod-Grain method)

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
22.08.2007 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -.46 at °C
pH value :
Method : other (calculated)
Year : 2007
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Experimental Database Structure Match: no data

SMILES : CCOP(S[Na])(=S)OCC
CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt
MOL FOR: C4 H10 O2 P1 S2 Na1
MOL WT : 208.21

Result : KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): -0.46

SMILES : CCOP(S[Na])(=S)OCC
CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt
MOL FOR: C4 H10 O2 P1 S2 Na1
MOL WT : 208.21

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	2	-CH2- [aliphatic carbon]	0.4911	0.9822
Frag	1	S=P [thio=phosphorus]	-0.6587	-0.6587
Frag	2	-O-P [aliphatic attach]	-0.0162	-0.0324
Frag	1	-S-P [sulfur, phosphorus attach]	0.6270	0.6270
Factor	1	misc-O-{Na,K,Li} [coef*(1+0.5*(NUM-1))]	-2.7000**	-2.7000
Const		Equation Constant		0.2290
NOTE		An estimated coefficient (**) used		

Log Kow = -0.4583

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
22.08.2007 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 97750 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Experimental Database Structure Match: no data

SMILES : CCOP(S[Na])(=S)OCC
CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt
MOL FOR: C4 H10 O2 P1 S2 Na1
MOL WT : 208.21

Result :

Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 9.775e+004 mg/L

SMILES : CCOP(S[Na])(=S)OCC
CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt
MOL FOR: C4 H10 O2 P1 S2 Na1
MOL WT : 208.21
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -0.46
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.46

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction (used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -0.328
Water Solubility at 25 deg C (mg/L): 9.775e+004

Reliability	:	(2) valid with restrictions

Modeled data

Flag	:	Critical study for SIDS endpoint

22.08.2007 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	
Conc. of sensitizer	:	
Rate constant	:	.0000000000916286 cm³/(molecule*sec)
Degradation	:	50 % after .1 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Method :

AOP Program (v1.92)
==========
SMILES : CCOP(S[Na])(=S)OCC
CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt
MOL FOR: C4 H10 O2 P1 S2 Na1
MOL WT : 208.21

Result :

AOP Program (v1.92) Results:
==========
-- SUMMARY (AOP v1.92): HYDROXYL RADICALS

Hydrogen Abstraction = 38.6286 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 53.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 91.6286 E-12 cm3/molecule-sec
HALF-LIFE = 0.117 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 1.401 Hrs
--- SUMMARY (AOP v1.91): OZONE REACTION

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi): 0.928
(Junge,Mackay)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Reliability	:	(2) valid with restrictions Modeled data
Flag	:	Critical study for SIDS endpoint

09.08.2007 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic

t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other (calculated)
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	HYDROWIN Program (v1.67): ========== SMILES : CCOP(S[Na])(=S)OCC CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt MOL FOR: C4 H10 O2 P1 S2 Na1 MOL WT : 208.21
Result	:	---------- HYDROWIN v1.67 Results ---------- Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!! ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!!
Reliability	:	(2) valid with restrictions Modeled data
Flag	:	Critical study for SIDS endpoint

22.08.2007 (3)

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Remark	:	: Hydrolysis is not expected to be a primary route of degradation based on analogy to Disulfoton (CAS 298-04-4). Disulfoton is stable to hydrolysis at 20o C at pH 5, 7, and 9, but hydrolyzes more rapidly at higher temperatures. Estimated hydrolysis half-lives for Disulfoton were 103 days at 25 ºC and pH 7 (Ellington et al. 1988) and 170 days at 11 ºC and pH 7.9 (Wanner et al. 1989).
Reliability	:	(2) valid with restrictions

22.08.2007 (2) (10) (11)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)

Soil : % (Fugacity Model Level II/III)
Method : other
Year : 2007

Method : Level III Fugacity Model (Full-Output):
==========

Chem Name : Phosphorodithioc acid, O,O-diethyl ester, sodium salt
Molecular Wt: 208.21
Henry's LC : 5.77e-014 atm-m3/mole (calc VP/Wsol)
Vapor Press : 2.06e-008 mm Hg (Mpbpwin program)
Liquid VP : 9.11e-008 mm Hg (super-cooled)
Melting Pt : 90.3 deg C (Mpbpwin program)
Log Kow : -0.46 (Kowwin program)
Soil Koc : 0.142 (calc by model)

Result : Level III Fugacity Model (Full-Output):
==========

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	8.79e-006	2.8	1000
Water	46.2	900	1000
Soil	53.7	1.8e+003	1000
Sediment	0.089	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.77e-017	0.0636	0.00257	0.00212	8.57e-005
Water	1.88e-018	1.04e+003	1.35e+003	34.7	45.1
Soil	7.98e-017	605	0	20.2	0
Sediment	1.8e-018	0.223	0.0521	0.00743	0.00174

Persistence Time: 976 hr
Reaction Time: 1.78e+003 hr
Advection Time: 2.16e+003 hr
Percent Reacted: 54.9
Percent Advected: 45.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 2.801
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.739 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
09.08.2007 (3)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	10.62
Elimination	:	
Method	:	other
Year	:	2007
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	BCF Program (v2.17) ========== SMILES : CCOP(S)(=S)OCC CHEM : Phosphorodithioc acid, O,O-diethyl ester, sodium salt MOL FOR: C4 H11 O2 P1 S2 MOL WT : 186.23
Result	:	BCF Program (v2.17) Results: ========== ---- Bcfwin v2.17 ---------- NOTE: Metals (Na, Li or K) are removed for BCF and log Kow evaluation! Log Kow (estimated) : 2.24 Log Kow (experimental): not available from database Log Kow used by BCF estimates: 2.24 Equation Used to Make BCF estimate: Log BCF = 0.77 log Kow - 0.70 + Correction Correction(s): Value No Applicable Correction Factors Estimated Log BCF = 1.026 (BCF = 10.62)
Reliability	:	(2) valid with restrictions Modeled data

09.08.2007 (3)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	310 - 330
Limit test	:	
Analytical monitoring	:	no data
Method	:	other
Year	:	1974
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : Fingerlings from three different egg sources were used. The fingerlings, ranged in weight 1-10 g were allowed to acclimate for 24 hours. 20 fish were added to each test aquaria. Approximately one hour after the fish were transferred, the sample (previously dissolved in an aliquot of experimental water) was added. Water temperature was maintained at 12 (+/-1) degree C. Median lethal oncentrations were determined by plotting median survival times, LC50, as a function of the logarithm of the concentration.
The experimental water used was naturally hard spring water used in a trout fish hatchery. The volume of water was adjusted to maintain a ratio of 2g wet fish per liter of water.

pH = 8.6;
total hardness = 348 ppm;
carbonate hardness = 203 ppm;
oxygen saturation was maintained by bubbling air into the water.

Result : LC50 = 400 - 410 ppm at 12 degrees C
LC50 = 310 - 330 ppm at 16 degrees C

Test substance : Phosphorodithioic acid, O,O-diethyl ester, sodium salt - Sodium Aerofloat (commercial product)

Reliability : (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment.

22.08.2007 (5)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	18100 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1991
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable Insufficient information to determine reliability.

09.08.2007 (1) (6)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2000 - mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	water
Doses	:	2000 mg/kg bw
Method	:	other: similar to OECD Guide-line 402
Year	:	1972
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The substance was applied undiluted to the skin of four rabbits. The skin of one male and one female animal was abraded. The animals were observed for 14 days for symptoms and mortality.
Result	:	Sex Dose # Deaths/# Symptoms/# exposed Male 2000 mg/kg 0/0/2 Female 2000 mg/kg 0/0/2 There were no clinical signs or deaths.
Test substance	:	sodium O,O-diethyl phosphorodithionate (CAS# 3338-24-7); commercial product; purity not indicated; 50% in water
Reliability	:	(2) valid with restrictions Similar to guideline study; not GLP
Flag	:	Critical study for SIDS endpoint

09.08.2007 (8)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	highly irritating
Classification	:	
Method	:	
Year	:	1991
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable Internal company data

09.08.2007 (1)

Species	:	rabbit
Concentration	:	
Dose	:	100 other: mg
Exposure time	:	24 hour(s)
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	moderately irritating
Classification	:	
Method	:	
Year	:	1986
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable Insufficient information to determine reliability.

09.08.2007 (6)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA98, TA100, TA1535, TA1537 and TA1538
Test concentration	:	100, 333, 1000, 3333 and 10,000 ug/plate
Cycotoxic concentr.	:	>10,000 ug/plate
Metabolic activation	:	with and without

Result : negative
Method : other: Ames
Year : 1986
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : The mutagenicity of Phosphorodithioic acid, O,O-diethyl ester, sodium salt was evaluated in Salmonella tester strains TA98, TA100, TA1535, TA1537 and TA1538 (Ames test), both in the presence and absence of Aroclor-induced rat liver S9 metabolic activation using the plate incorporation technique.

Preliminary toxicity determination: The salmonella/mammalian microsome mutagenicity assay is divided into two phases. The first phase, the preliminary toxicity determination, is used to establish the dose range over which the test article will be assayed. The second phase is the mutagenicity assay of the test article. In the preliminary assay, strain TA 100 was diluted in water and dosed at 10, 33.3, 66.7, 100, 333.3, 666.7, 1,000, 3333.3, 6666.7, and 10,000 ug/plate with and without metabolic activation.

Definitive assay:
Five doses of the test article in DMSO (100, 333, 1000, 3333 and 10,000 ug/plate) were plated with all five tester strains with and without metabolic activation. All solvent controls and test article doses were plated in triplicate. The plates were incubated for 48-72 hours at 37 +/- 3 deg C.

Positive controls were included:
Without S9 activation: Sodium azide (5 ug/plate); 9-Aminoacridine (75 ug/plate); 2-Nitrofluorene (5 ug/plate)
With S9 activation: 2-Anthramine (4 ug/plate)

Result : Preliminary assay: The results of the preliminary toxicity determination indicated that the appropriate maximum dose level to be tested in the mutagenicity assay would be 10,000 ug/plate with and without metabolic activation.

Definitive assay: Positive control plates and TA 1537 were hand counted and manually entered into the computer. The other experimental plates were machine counted and automatically entered into the computer. Mean summary data are presented below:

Dose	S9	Salmonella strains (revertants/plate)				
		TA1535	TA1537	TA1538	TA98	TA100
100	(-)	19	7	16	17	98
333	(-)	28	5	12	16	110
1000	(-)	19	5	16	25	100
3333	(-)	26	4	14	19	103
10000	(-)	22	8	16	18	117
100	(+)	15	7	25	35	136
333	(+)	17	9	23	36	124
1000	(+)	15	9	18	36	114
3333	(+)	14	9	24	31	123
10000	(+)	18	8	23	30	107

Test substance : Phosphorodithioic acid, O,O-diethyl ester, sodium salt; Lot number CLS-1;4; CAS No. 3338-24-7; purity 48%
Conclusion : Under the conditions of the study, the test material did not cause a positive response in any of the tester strains with or without metabolic activation by Aroclor-induced rat liver microsomes.
Reliability : (1) valid without restriction
Guideline study

17.08.2007 (4)

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) BAYER CORPORATION (1991) MSDS Diethyl Salt Solution AGRICULTURE DIVISION P.O. Box 4913 Hawthorn Road Kansas City, MO 64120-0013

(2) Ellington JJ, Stancil FE, Payne WD, et al. 1988. Measurement of hydrolysis rate constants for evaluation of hazardous waste land disposal: Vol. 3. Data on 70 chemicals. Engineering Research Laboratory, U.S. Environmental Protection Agency, Athens, GA. EPA/600/S3-88-028. NTIS PB38-234842/AS. Cited in ATSDR Toxicological Profile for Disulfoton (1995) http://www.atsdr.cdc.gov/toxprofiles/tp65.html#bookmark12

(3) EpiWin v.3.11 (2007)

(4) FMC Corporation (1986) Phosphorodithioic acid, O,O-diethyl ester, sodium salt: Salmonella/Mammalian-Microsome Plate Incorporation Mutagenicity Assay (Ames Test). Study Number A85-1802. Fiche Number: 0000465-1 Cited in NISC BiblioLine

(5) Fuerstenau MC, Wakawa BM, et al. (1974). Toxicity of selected sulfhydryl collectors to rainbow trout. Transactions. Society of Mining Engineers. 256(4): 337-341.

(6) Marhold, J. (1986). "Prehled Prumyslove Toxicologie; Organicke Latky." p 1175. Prague, Czechoslovakia, Avicemun. as reported in NISC BiblioLine.

(7) McEwen, W.E (1982) Phosphorus and Sulfur and the Related Elements, 1982, W 13(1), p 35-40.

(8) Mobay Chemical Corporation. (1972). CHEMAGRO Agricultural Division Study Report No. 35287

(9) NISC (2007) BiBlioLine

(10) Patterson, M (2003) Disulfoton Analysis of Risks to Endangered and Threatened Salmon and Steelhead. USEPA, Environmental Field Branch Office of Pesticide Programs. http://www.epa.gov/oppfead1/endanger/effects/disulfoton-analysis.pdf

(11) Wanner U, Egli, T., Fleischmann T, et al. 1989. Behavior of the insecticides disulfoton and thiometon in the Rhine River.A chemodynamic study. Environmental Science and Technology 23:1232-1242. Cited in ATSDR Toxicological Profile for Disulfoton (1995) http://www.atsdr.cdc.gov/toxprofiles/tp65.html#bookmark12

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT